

*Abstracted/indexed in: Chemical Abstracts, ERDA Abstracts, ISI Current Contents, Inspec Abstracts, Nuclear Engineering Abstracts, Physics Abstracts, Physikalische Berichte/Physics Briefs*

- Ab initio investigation of the potential energy surfaces involved in the photophysics of *s-trans*-1,3-butadiene  
B. Ostojić and W. Domcke 1
- The additivity of the  $\pi$ -electron correlation energy in planar heteroatomic molecules  
Z.B. Maksić, D.M. Smith and D. Barić 11
- Potential coupling of intramolecular to intermolecular modes: an ab initio study of the amino inversion and van der Waals motions in the aniline-argon complex  
I. López-Tocón, J.C. Otero, M. Becucci, G. Pietraperzia, E. Castellucci and P. Bréchignac 29
- Reduced dimensionality quantum reactive scattering calculations on the ab initio potential energy surface for the  $O(^1D) + N_2O \rightarrow NO + NO$  reaction  
T. Takayanagi and A. Wada 37
- A theoretical study on electron donor-acceptor complexes of  $Et_2O$ ,  $Et_2S$  and  $Me_3N$  with interhalogens,  $I-X$  ( $X = Cl$  and  $Br$ )  
S.P. Ananthavel and M. Manoharan 49
- Hydrogen bonding in picolinic acid *N*-oxide. Part II: A proposal for dissipative laser driven proton transfer dynamics  
N. Došlić, J. Stare and J. Mavri 59
- Calculation of  $^{14}N$  and  $^{35}Cl$  quadrupole coupling constants on optimized molecular structures of pyrimidine, 2-*X*- and 5-*X*-pyrimidine, with  $X = F, Cl, Br$ , and  $CN$   
W.C. Bailey 75
- Absorption spectra of the GFP chromophore in solution: comparison of theoretical and experimental results  
A.A. Voityuk, A.D. Kummer, M.-E. Michel-Beyerle and N. Rösch 83
- The influence of the stretch modes on the classical highly excited bend motion with Darling-Dennison coupling in acetylene  
G. Wu 93
- An investigation of the HOMO frontier orbital electron density distributions of  $NH_3$ , the methylamines and  $NF_3$  using DFT and electron momentum spectroscopy  
C.E. Brion, J.B. Young, I.V. Litvinyuk and G. Cooper 101
- Non-orthogonal orbitals for localized electrons III. Application to periodic one dimensional lattices  
G. Bignonneau, A. Fritsch and L. Ducasse 107

(continued on inside back page)



0301-0104(20010701)269:1-3;1-P



<http://ChemWeb.com>  
The World Wide Club for the Chemical Community

Abstracted/indexed in: Chemical Abstracts, ERDA Abstracts, ISI Current Contents, Inspec Abstracts, Nuclear Engineering Abstracts, Physics Abstracts, Physikalische Berichte/Physics Briefs

- Ab initio investigation of the potential energy surfaces involved in the photophysics of *s-trans*-1,3-butadiene  
B. Ostojić and W. Domcke 1
- The additivity of the  $\pi$ -electron correlation energy in planar heteroatomic molecules  
Z.B. Maksić, D.M. Smith and D. Barić 11
- Potential coupling of intramolecular to intermolecular modes: an ab initio study of the amino inversion and van der Waals motions in the aniline-argon complex  
I. López-Tocón, J.C. Otero, M. Becucci, G. Pietraperzia, E. Castellucci and P. Bréchignac 29
- Reduced dimensionality quantum reactive scattering calculations on the ab initio potential energy surface for the  $O(^1D) + N_2O \rightarrow NO + NO$  reaction  
T. Takayanagi and A. Wada 37
- A theoretical study on electron donor-acceptor complexes of  $Et_2O$ ,  $Et_2S$  and  $Me_3N$  with interhalogens,  $I-X$  ( $X = Cl$  and  $Br$ )  
S.P. Ananthavel and M. Manoharan 49
- Hydrogen bonding in picolinic acid *N*-oxide. Part II: A proposal for dissipative laser driven proton transfer dynamics  
N. Došlić, J. Stare and J. Mavri 59
- Calculation of  $^{14}N$  and  $^{35}Cl$  quadrupole coupling constants on optimized molecular structures of pyrimidine, 2-*X*- and 5-*X*-pyrimidine, with  $X = F, Cl, Br$ , and  $CN$   
W.C. Bailey 75
- Absorption spectra of the GFP chromophore in solution: comparison of theoretical and experimental results  
A.A. Voityuk, A.D. Kummer, M.-E. Michel-Beyerle and N. Rösch 83
- The influence of the stretch modes on the classical highly excited bend motion with Darling-Dennison coupling in acetylene  
G. Wu 93
- An investigation of the HOMO frontier orbital electron density distributions of  $NH_3$ , the methylamines and  $NF_3$  using DFT and electron momentum spectroscopy  
C.E. Brion, J.B. Young, I.V. Litvinyuk and G. Cooper 101
- Non-orthogonal orbitals for localized electrons III. Application to periodic one dimensional lattices  
G. Bignonneau, A. Fritsch and L. Ducasse 107

(continued on inside back page)



0301-0104(20010701)269:1-3;1-P



<http://ChemWeb.com>  
The World Wide Club for the Chemical Community

## Contents

(continued from outside back cover)

Five-coordinate nitrosyl iron(II) tetraphenylporphyrin exhibits porphyrin ring $^{14}\text{N}$ symmetry about the Fe-N-O plane: a hyperfine sublevel correlation spectroscopy study D.C. Gilbert and D.C. Doetschman	125
Finite-field Møller-Plesset perturbation theory and coupled cluster calculations of the electric multipole moments and the dipole polarizability of $\text{As}_2$ G. Maroulis and P. Karamanis	137
Degeneracy, orientational disorder and chromophore size effects on Frenkel excitons in columnar mesophases D. Markovitsi, L.K. Gallos, J.P. Lemaistre and P. Argyrakis	147
Core excitation and autoionising transitions from $1,3\Pi_u$ states of $\text{N}_2$ , by near threshold electron impact D.P. Almeida, G. Dawber, S.E. Michelin and G.C. King	159
Chemical generation of atomic iodine for chemical oxygen-iodine laser. I. Modelling of reaction systems V. Jirásek, O. Špalek, J. Kodymová and M. Čenský	167
A theoretical study of the reaction of hypochlorous acid with the bromite ion S. Guha and J.S. Francisco	179
Equilibrium dimer concentrations in gases and gas mixtures J.W. Eerkens	189
Molecular dynamics studies of phase transition of KI clusters X.-l. Zhu, X.-z. You, R.-g. Xiong and Z. Zhou	243
On electrostatics of extended multiphonon transitions and nature of the J-band V.V. Egorov	251
Vapor-liquid equilibria of dendrimer solutions: the effect of endgroups at the periphery of dendrimer molecules J.G. Jang and Y.C. Bae	285
A Monte Carlo simulation study of solvent effect on $\text{Eu}^{3+}$ to $\text{Nd}^{3+}$ ion mutation H.-S. Kim	295
Ultrasonic studies of dynamics of critical concentration fluctuations in benzonitrile-isooctane mixture T. Hornowski and D. Madej	303
Thermally induced spectral diffusion of Rhodamine 3B in viscous polyols J.A.B. Ferreira and S.M.B. Costa	313
Higher excited state fluorescence of mixed ligand lanthanide(III) complexes with acetylacetonato, nitrate and terpyridine M. Hasegawa, A. Nakao, M. Masui, T. Tamura, D. Suzuki, W. Linert, Y. Fukuda and T. Hoshi	323
Photophysical properties of pheophorbide- <i>a</i> -substituted diaminobutane poly-propylene-imine dendrimer S. Hackbarth, V. Horneffer, A. Wiehe, F. Hillenkamp and B. Röder	339
Diagnosis of a benzene discharge with a mass-selective spectroscopic technique F. Güthe, H. Ding, T. Pino and J.P. Maier	347

(continued on preceding page)

## Contents

*(continued from following page)*

Characterization of bisazo compounds employing ultrafast spectroscopy R. Karpicz, V. Gulbinas, A. Stanishauskaite and A. Undzenas	357
Decay dynamics of interchain excited states in luminescent conjugated polymer CN-PPV J.-H. Hsu, W. Fann, H.-F. Meng, E.-S. Chen, E.-C. Chang, S.-A. Chen and K.-W. To	367
Solid-state optical properties of the methyl-exopyridine-anthracene rotaxane G. Gadret, R. Zamboni, P. Schouwink, R.F. Mahrt, J. Thies, T. Loontjens and D.A. Leigh	381
The collisional quenching of $\text{CCl}_2(\text{A}^1\text{B}_1 \text{ and } \text{a}^3\text{B}_1)$ by substituted methane molecules Y. Gao, Y. Chen, X. Ma and C. Chen	389
Microstructure of indocyanine green J-aggregates in aqueous solution J. Zweck and A. Penzkofer	399
Cobalt valence tautomeric compounds: molecular and solid state properties S. Klokishner	411
Theoretical study TPA properties of a series of two-dimensional charge-transfer derivatives Y.-f. Zhou, F.-q. Meng, X. Zhao, S.-y. Feng and M.-h. Jiang	441
Author index	447
Subject index	451
Instructions to authors	463

---

**CONTENTS**  
**direct**

This journal is part of **ContentsDirect**, the *free* alerting service which sends tables of contents by e-mail for Elsevier Science books and journals. You can register for **ContentsDirect** online at: [www.elsevier.nl/locate/contentsdirect](http://www.elsevier.nl/locate/contentsdirect)

---

